Layering in Crumpled Sheets

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Abstract

We introduce a toy model of crumpled sheets. We use simulation to show there is a first order phase transition in the model, from a disordered dilute phase to a mixture with a layered phase.

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I. INTRODUCTION

When a sheet of stiff paper is crumpled into a compact ball, creases and folds appear. This storage of energy, especially in the irreversibly distorted creases, has been widely studied, for instance in [1–4]. Our interest here is in geometric changes associated with the (reversible) folds, which is less well understood. See for instance [5,6].

Consider the densest possible state of the material, in which the sheet is carefully folded into a compact stack of parallel leaves. (There needs to be a significant cost for bending the material or else dense packings will usually be more complicated.) Imagine the process of compactifying the sheet within a contracting sphere, from a typical initial state of low volume fraction near 0 to a typical state of high volume fraction near 1. How would such a process proceed? For a material in thermal equilibrium there is a pair of first order phase transitions associated with quasistatic compactification; low density configurations are of random character (fluid), while high density configurations are ordered (solid), and isothermal compactification would progress between these extremes via freezing and then melting transitions, separated by phase coexistence in which the material consists of macroscopic portions of each phase. Our computations, in a toy model, suggest that compactification of a stiff sheet undergoes a similar path, at least from its low volume fraction disordered state to a reorganization of the state into an inhomogeneous intermediary (part random and part folded), as is typical of freezing.

Our toy model is not of a thin, stiff sheet in three dimensions but of a thin, stiff wire loop in two dimensions, which we expect to behave similarly [7]. (Confined wire in three dimensions may well behave differently; see for instance [8].) In the model the wire is restricted to a triangular lattice, so a configuration in the model is a self-avoiding closed walk (loop) on the lattice, with energies associated to bends in the walk to penalize the bends.

II. THE MODEL AND RESULTS

For a fixed integer n consider the triangular lattice $L = \{(a + b/2, b\sqrt{3}/2) : (a, b) \in (\mathbb{Z}/n\mathbb{Z})^2\}$ with periodic boundary conditions. Note that this space is homogeneous and isotropic.

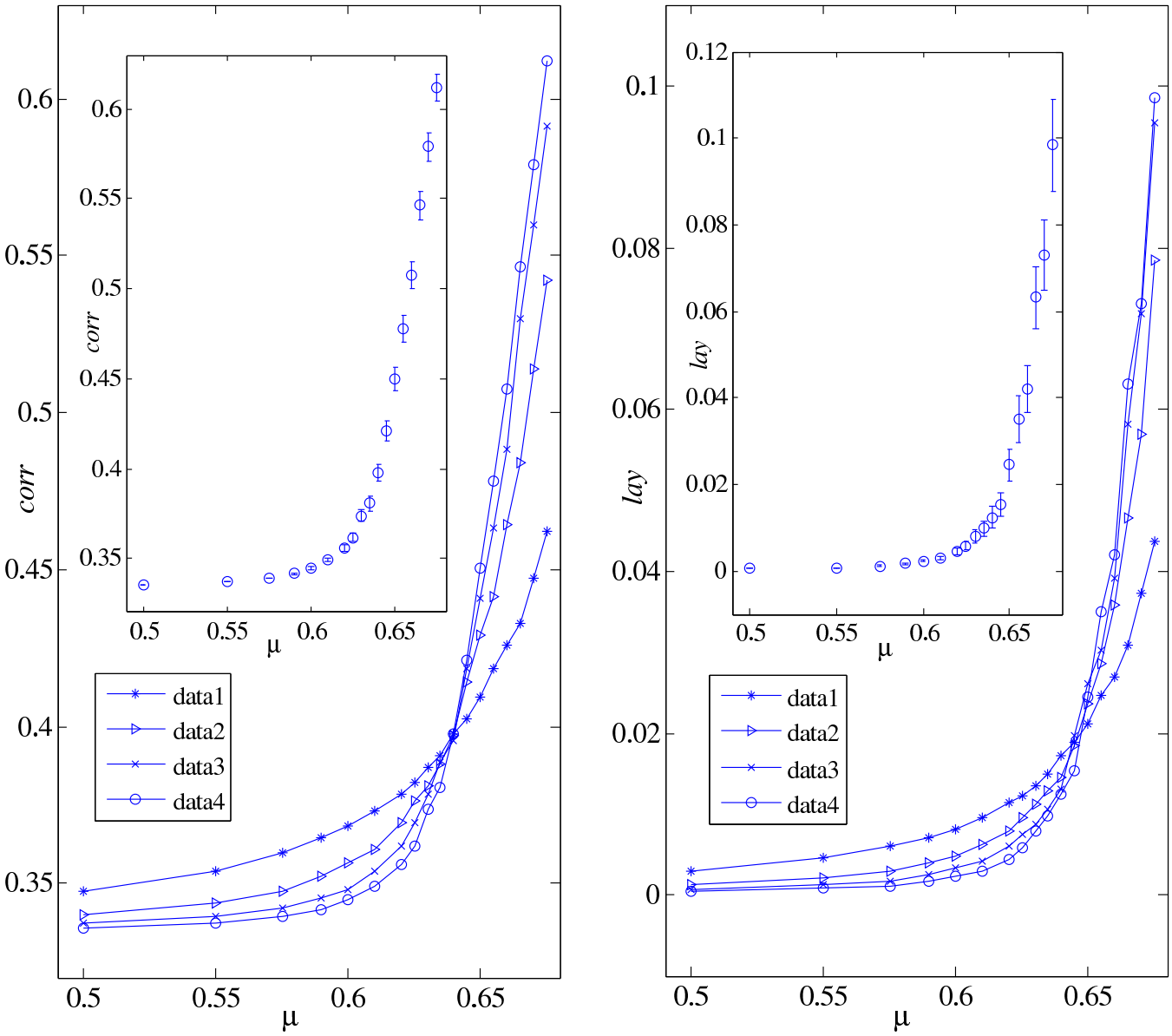

FIG. 1: a) Correlation vs. mu, for volumes 40^2 (data1) through 100^2 (data4); b) Layer size vs. mu, for volumes 40^2 (data1) through 100^2 (data4). Error bars in both insets represent 95% confidence intervals for volume 100^2, and for low μ are smaller than the data circles.

Let $\mathcal{A}$ be the set of oriented self-avoiding closed walks on L, its elements being called *configurations*. If a walk $C \in \mathcal{A}$ changes direction at a vertex, we say there is a bend there. If it changes by $\pm\pi/3$, we call the bend large; if it changes by $\pm\pi/6$ we call it small. We define $B_s(C)$ as the number of small bends in C and $B_\ell(C)$ as the number of large bends in C. Assigning the energy e_s to each small bend and e_ℓ to each large bend, we define the

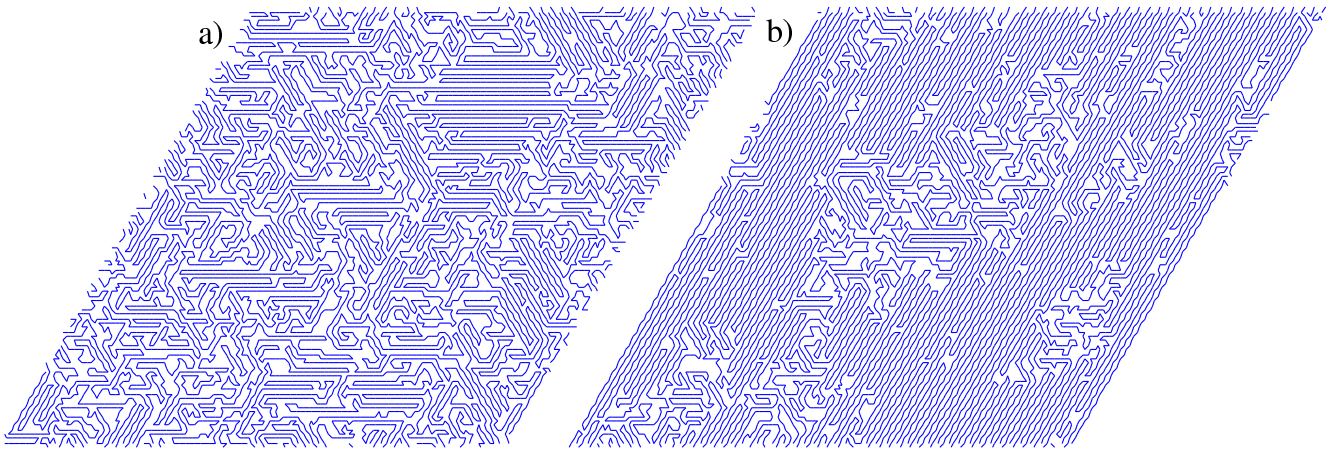

FIG. 2: Snapshots of a loop in available volume 100^2 in equilibrium at $\mu = 0.6$ in a), and $\mu = 0.67$ in b).

total energy of configuration C by:

$$\mathcal{E}(C) = B_s(C)e_s + B_\ell(C)e_\ell, \tag{1}$$

and denote the model with energy parameters e_s and e_ℓ by $e_s : e_\ell$.

Because it is harder to simulate our model at fixed density and/or fixed energy, we use conjugate variables β for energy $\mathcal{E}$ and μ for particle (edge) number N, assigning the probability $m_\mu(C)$ for any $C \in \mathcal{A}$:

$$m_\mu(C) = \frac{e^{-\beta[\mathcal{E}(C)-\mu N(C)]}}{Z}, \tag{2}$$

where Z is the normalization. (We suppress dependence on the system size.) We take $\beta = 1$ without loss of generality, so that the variable parameters in our model are μ and the energies of the two bending angles, e_ℓ and e_s. We have simulated $1:2$ and $1:\infty$, with qualitatively similar results; here we state results only for $1:2$.

To simulate the $1:2$ model at μ-values $\mu_0 < \mu_1 < ... < \mu_{l-1}$, we start with $\mu = \mu_0$ and a configuration which is a cycle with 6 edges. The end configuration in the simulation of μ_i is taken as the starting configuration in the simulation of μ_{i+1}. The basic Monte Carlo step is: pick at random either an edge e_1 or a pair of intersecting edges e_2, e_3, and then replace e_1 with a pair of intersecting edges e_2', e_3', or replace e_2, e_3 with an edge e_1', with probabilities determined by m_{μ_i}, such that the resulting configuration is legal (i.e. is a self-avoiding closed loop).

For each measurement *meas* we use a standard autocorrelation function to find a "mixing time" at each μ_i, which we define as the smallest value of t such that the autocorrelation

$$A(t) := \frac{1}{(m-t)\sigma^2} \sum_{i=1}^{m-t} (meas(C_i) - \mu) \cdot (meas(C_{i+t}) - \mu) \tag{3}$$

falls below zero. Here $C_1, ..., C_m$ is the Monte Carlo chain corresponding to the simulation of μ_i, and μ and σ^2 are the (sample) average and variance of *meas* over that chain. We found that for each of our measurements *meas* (described below), our simulations of each μ_i were on average at least 20 times as long as the corresponding mixing times. We therefore believe our simulations are in equilibrium at each μ_i. We obtain error bars from the Student's t-distribution by running 200 independent copies of the simulation.

We make the following measurements to detect the spontaneous symmetry breaking and layering which may occur at large μ. We first consider a correlation measurement $corr(C)$: choose a random edge in C and define $corr(C)$ as the proportion of edges in C which are parallel to it. Since the model is isotropic we expect $corr(\mu)$ to be identically $1/3$ for small μ in the infinite volume limit.

To detect bulk-sized layers, that is, layers proportional to the size of the system, we define $lay(C)$ as the size of the largest 80% perfect square "layer" centered at the origin in C, divided by the system size. (Perfect means no bends.) We expect that for small μ, *lay* is identically zero in the infinite volume limit. Note that the choice of 80% is rather arbitrary; any percentage significantly above 33% should detect bulk layers.

The data gives strong evidence of a phase transition, namely that in the infinite volume limit $corr(\mu)$ is identically $1/3$ for $\mu < \mu^*$ and $corr(\mu) > 1/3$ for $\mu > \mu^*$, where $\mu^* \approx 0.63$. See Figure 1a, with error bars in the inset. The data in Figure 1 are performed on systems of volume: $40^2 = 1600,\ 60^2 = 3600,\ 80^2 = 6400$ and $100^2 = 10,000$.

As further detail of the nature of the ordered phase signalled by *corr*, the data displayed in Figure 1b, computed in the same family of simulations, suggests that in the infinite volume limit *lay* is identically zero below μ^*, but positive above μ^*, showing the emergence of bulk layers above μ^*. The transition can be seen in configuration snapshots; see Figure 2. We also measure volume fraction, $\phi(\mu)$. The data in Figure 3 suggests that in the infinite volume limit a discontinuity develops in the slope of $\phi(\mu)$ at μ^*, in accord with the other evidence of a transition.

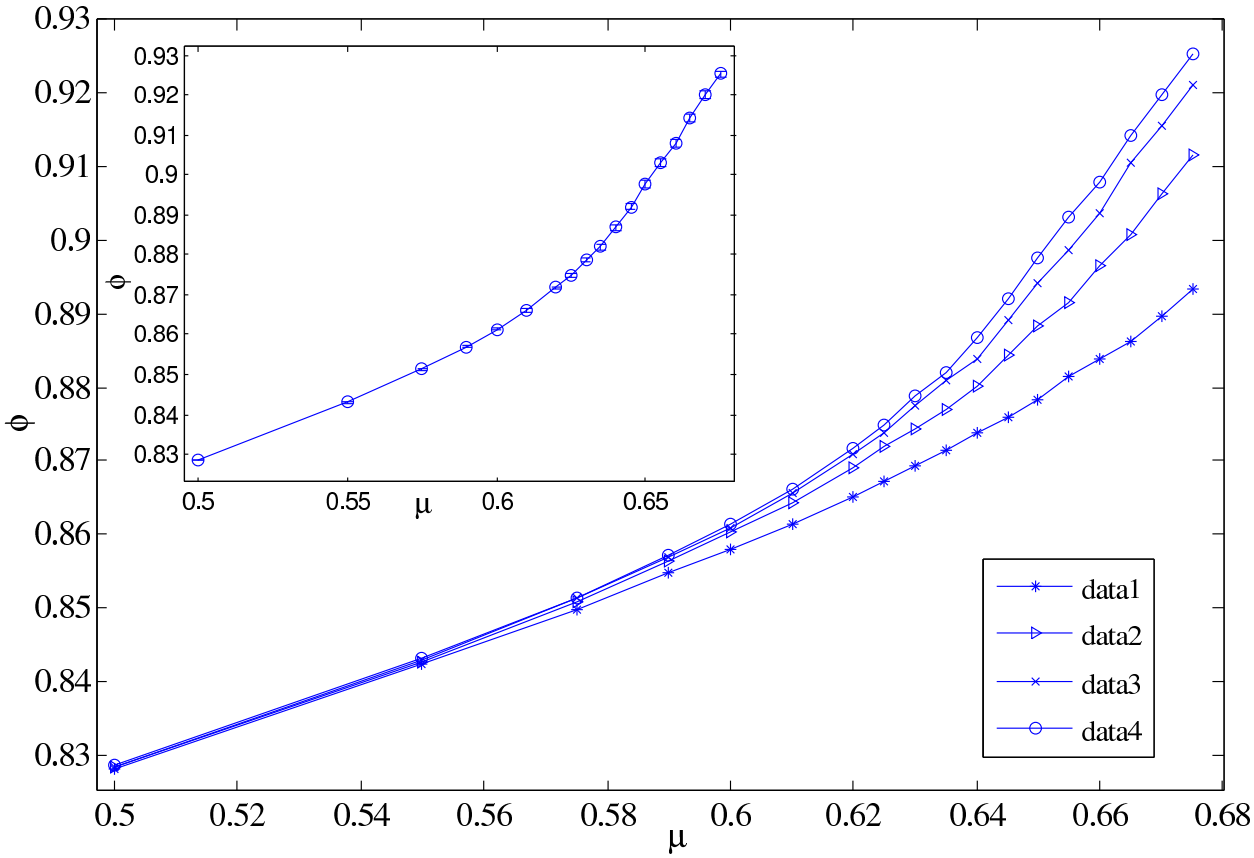

FIG. 3: Volume fraction vs. mu, for volumes 40^2 (data1) through 100^2 (data4). Error bars in the inset figure represent 95% confidence intervals for volume 100^2, and are mostly smaller than the data circles.

III. SUMMARY

We have introduced and simulated a toy model for the folding of progressively confined stiff sheets. We find that bulk folding emerges at a sharp volume fraction as the material is compacted, just as bulk solids form at a sharp volume fraction in the freezing transition of equilibrium fluids. This analogy has previously been used to model the behavior of other types of soft matter, in particular colloids [9] and the random close packing of granular matter [10,11].

We note an old model due to Flory [12] which has been applied to crumpled materials; see [13] and references therein. In that two dimensional lattice model one varies the temperature with volume fraction fixed at one. There is general agreement that it exhibits a phase transition, perhaps representing the melting of a dense ordered phase. This melting

transition is usually characterized as continuous (second order), though this is sometimes disputed [13].

The phase transition we find in our model should be experimentally verifiable, in both compacted stiff sheets and in two dimensionally confined compacted stiff wires.

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